Parameter Selections in Simulating the Physical Diffusion Phenomena of Suspended Load by Low-Order Differential Scheme Numerical Dispersion

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Abstract

In this paper, the process of the introduction of numerical diffusion is investigated when low-order differential scheme in convection-diffusion equation for discrete suspended load is in use. According to the results of instances calculation, the optimal choice for parameters when physical diffusion is simulated by numerical diffusion is obtained. Finally, comparison between several commonly used low-order schemes is conducted and the most viable low-order scheme in simulating physical diffusion by numerical diffusion is proposed in dealing with suspended load.

Keywords

Differential Scheme; Convection-Diffusion Equation of Suspended Load; Numerical Diffusion

Introduction

In general, using the low-order scheme for numerical calculations will more or less introduce numerical diffusion (Xie 1990). Different schemes have varying degrees of numerical diffusion. In theory this is not conducive to the exact solution of numerical calculation, but utilizing the numerical diffusion, such as to simulate the physical diffusion phenomenon, is also an effective method (Yang 1993). As for how to use the numerical diffusion to simulate the physical diffusion, and how to select parameters to achieve an acceptable level of the simulation results, they are the issues to be discussed in this paper.

Convection-Diffusion Equation for One-Dimensional Suspended Load

Equation for suspended load movement is (Zheng and Zhao 2001):

$$\frac{\partial AS}{\partial t}+\frac{\partial QS}{\partial x}-\frac{\partial}{\partial x}AD_x\frac{\partial S}{\partial x}=(S-r^{'})\frac{\partial A_S}{\partial t}$$

Introducing the flow continuity equation, the equation above can be rewritten as:

$$\frac{\partial S}{\partial t}+\frac{Q}{A}\frac{\partial S}{\partial x}-\frac{1}{A}\frac{\partial}{\partial x}AD_x\frac{\partial S}{\partial x}=\frac{(S-r^{'})}{A}\frac{\partial A_S}{\partial t}$$

where D_x the longitudinal diffusion coefficient, for sediment diffusion, it can be approximated as

$$D_x=0.25u_*h$$

Generally, for transportation issue of suspended load, the longitudinal diffusion of suspended load is much smaller than the longitudinal conviction of sediment, which is often overlooked. If the carrier velocity and diffusion coefficient D_x are constants without considering the source item, the convection-diffusion equation will be

$$\frac{\partial S}{\partial t}+u\frac{\partial S}{\partial x}=D_x\frac{\partial^2 S}{\partial x^2}$$

For this equation, the main numerical difficulty is to calculate the convection term because it strictly demands the conservation of matter, while the differential method for numerical solution often cannot achieve this. If the solution to convection-diffusion is considered under the premise of a good solution to convection-diffusion term, the probability of successful numerical solution would be higher. If ignoring the diffusion term, we can get the pure convection equation

$$\frac{\partial S}{\partial t}+u\frac{\partial S}{\partial x}=0$$

Establishment of Differential Scheme

Select Upwind scheme discrete pure convection equation, when $u>0$, the differential equation is (Courant 1928)

$$S_j^{n+1}=S_j^n-C_r(S_j^n-S_{j-1}^n)$$

where C_r is Crout number and $C_r=\widetilde{C}\Delta t/\Delta x$

The differential equation can be reduced to

$$\frac{S_j^{n+1}-S_j^n}{\Delta t}+\widetilde{C}\frac{S_j^n-S_{j-1}^n}{\Delta x}=0$$

The first item in the above equation is the forward difference quotient of $\partial S/\partial t$, and the second term is backward difference quotient of $\partial S/\partial t$, then $\widetilde{C}=u$ can be drawn. We will exam the compatibility, stability and convergence of the scheme as follows. Expand S_j^{n+1} and S_{j-1}^n on point (j,n)

$$S_j^{n+1}=S_j^n+(\frac{\partial S}{\partial t})_t^n\Delta t+\frac{1}{2}(\frac{\partial^2 S}{\partial t^2})_j^n\Delta t^2+...$$

$$S_{j-1}^n=S_j^n-(\frac{\partial S}{\partial x})_j^n\Delta x+\frac{1}{2}(\frac{\partial^2 S}{\partial x^2})_j^n\Delta x^2+...$$

Take them into the differential equation, and use the pure convection equation to get

$$\frac{\partial S}{\partial t}+u\frac{\partial S}{\partial x}=\frac{\Delta x^2 C_r(1-C_r)}{2\Delta t}\frac{\partial^2 S}{\partial x^2}$$

Assume $D_n=\dfrac{\Delta x^2 C_r(1-C_r)}{2\Delta t}$

Then $\dfrac{\partial S}{\partial t}+u\dfrac{\partial S}{\partial x}=D_n\dfrac{\partial^2 S}{\partial x^2}$

Comparing to the pure convection equation, only the right term of the equation tends to be zero when the space and time step are small enough, which means they are compatible. Taking $\Delta t=C_r\Delta x/C$ into D_n, we can get $D_n=\dfrac{\Delta x C(1-C_r)}{2}$

where $C=u$, $0<C_r<1$, when $\Delta x\to 0$, $\Delta t\to 0$, and $D_n=0$. So the difference equations and differential equations are compatible, as the stability condition for Upwind is $\left|u\right|\Delta t/\Delta x\le 1$. Using Lax equivalence theorem again we can get that the solution of differential equation converges to the solution of differential equations.

From the above proof it is clear that, Upwind scheme disperses a pure convection equation and an equation similar to convective diffusion can be obtained. Although the differentiated items $D_n\partial^2 S/\partial x^2$ can make the equation compatible, calculation shows that the item also makes the solution of differential equations no longer converge to the solution of the original differential equation. Instead it converges to the solution of the convection-diffusion equation, which means the implicit numerical diffusion, resulting from the limitation of Δx, Δt, which cannot be infinitely close to zero. However, since it is known that difference equations converge to the convection-diffusion equation, then it is used to identify the required parameter values, so that the differential equations can converge precisely to differential equations, namely numerical diffusion can simulate the physical diffusion well.

The Instance Analysis of Parameters Effect

As differential equation is similar in form with convection-diffusion equation, D_n might be called numerical diffusion coefficient. It is clear that the closeness between numerical diffusion coefficient D_n and physical diffusion coefficient D_x can determine the accuracy of the numerical diffusion in simulating physical diffusion, thus the problem is to find the right parameters, so that D_n can be close to D_x (Papadakis and Metaxas 2011). On the other hand, three parameters can determine D_n which are velocity u, space interval Δx and time step Δt, where flow rate should be in accordance with the actual engineering value, and Δx is subject to the restrictions on the boundary simulation accuracy (it will take on different values in accordance with the different size of the project and the complexity of the border. Usually, for example, the smaller the size of Δx is, the more precise the boundary simulation results will be. But it will increase the amount of calculation), only the time step Δt has wider choice. By selecting different Δt we can get the corresponding numerical diffusion coefficient D_n. Then comparing D_n with different longitudinal diffusion coefficient D_x, the impact of Δt on calculated results can be examined (Gasiorowski 2013).

Build the following model:

Model 1

Length is 10km, width is 2m, water depth is 4m, Chezy coefficient C is 25, and flow rate is 0.5m/s, Δx =200m. Take respectively Δt =400s, 399.5s, 399s, 360s, 300s, 200s…

The calculation results are shown as follows (Table 1).

TABLE 1 CALCULATION RESULTS (U=0.5M/S)

Δt (s)	Parameters		
	C_r	D_n	D_x
400	1	0	0.063246
399.5	0.99875	0.0625	0.063246
399	0.9975	0.125	0.063246
360	0.9	5	0.063246
300	0.75	12.5	0.063246
200	0.5	25	0.063246
100	0.25	37.5	0.063246
50	0.125	43.75	0.063246
0.5	0.00125	49.9375	0.063246

In the above table, only when Δt =399.5s, the difference between numerical diffusion coefficient D_n and longitudinal diffusion coefficient D_x is the smallest at 0.000746. At the same time, the difference between C_r and 1 is 0.00125, when Δt decreases by 0.5s to 399s. The two diffusion coefficients differs in an order of magnitude, indicating that only when C_r is very close to 1 the physical diffusion can be simulated more accurately. On the other hand, the numerical diffusion coefficient D_n will increase with the decrease of C_r. When C_r tends 0, a solution with larger error will be got.

Here the time step is accurate to the extent of 0.5, which is not conducive to calculation. Since the time step may be influenced by the flow velocity, the flow rate is changed and the model is modified as follows:

Model 2

Flow velocity u =1m/s, taking Δt =400s, 300 s 200s, 199.5s, 199s, 198s… other parameters are unchanged.

In the results (Table 2) when Δt is greater than Δx, numerical diffusion coefficient is negative. It will repeat the last calculation law when they are equal. In fact if the formula is changed for D_n, we can find the contradictions.

$$D_n = \frac{\Delta x^2 C_r(1-C_r)}{2\Delta t} = \frac{u\Delta x - u^2\Delta t}{2}$$

When u =1m/s, $D_n = (\Delta x - \Delta t)/2$, obviously Δx needs to be larger than Δt to make D_n positive, in fact, this is caused by the failure to satisfy the stability condition $|u|\Delta t/\Delta x \le 1$. And, from another perspective, the accuracy of D_n shows direct linear relationship with the precision of Δx as well as Δt, which demands highly for Δx and Δt, in the actual calculation, it is often impossible to meet such a request, so other flow rates should be taken to calculate again.

TABLE 2 CALCULATION RESULTS (U=1M/S)

Δt (s)	Parameters		
	C_r	D_n	D_x
400	2	-100	0.126491
300	1.5	-50	0.126491
200	1	0	0.126491
199.5	0.9975	0.25	0.126491
199	0.995	0.5	0.126491
198	0.99	1	0.126491
100	0.5	50	0.126491
50	0.25	75	0.126491
0.5	0.0025	99.75	0.126491

Model 3

Flow velocity u =0.8m/s, taking Δt =250s, 249.5s, 249s, 200s, 100s, 50s… The remaining parameters are unchanged.

Model 4

Flow rate u =0.2m/s, taking Δt =1000s, 999.5s, 999s, 998s, 900s, 800s… The remaining parameters are unchanged.

Calculation results are shown in Table 3 and Table 4 respectively.

TABLE 3 CALCULATION RESULTS (U=0.8M/S)

Δt **(s)**	**Parameters**		
	C_r	D_n	D_x
250	1	0	0.101193
249.5	0.998	0.16	0.101193
249	0.996	0.32	0.101193
200	0.8	16	0.101193
100	0.4	48	0.101193
50	0.2	64	0.101193
0.5	0.002	79.84	0.101193

TABLE 4 CALCULATION RESULTS (U=0.2M/S)

Δt **(s)**	**Parameters**		
	C_r	D_n	D_x
1000	1	0	0.025298
999.5	0.9995	0.01	0.025298
999	0.999	0.02	0.025298
998	0.998	0.04	0.025298
900	0.9	2	0.025298
800	0.8	4	0.025298
500	0.5	10	0.025298
100	0.1	18	0.025298
0.5	0.0005	19.99	0.025298

Combining the above four models; we can draw the following rules:

- When u is in the interval (0,1], the longitudinal diffusion coefficient D_x increases as u increase, and the maximum value is close to 0.126 (this is the maximum value when the water depth is 4m and Chezy coefficient is 25, depending on the circumstances, the value will be different);
- When u is in the interval (0,1], if u is small, the numerical diffusion simulation of physical diffusion is better, which is the closest when u =0.5m/s;
- When u is in the interval (0,1], the simulation is better when the time step value is 0.5s smaller than the "Δt that makes C_r =1", but the difference of 0.5s is not ideal;
- When u is in the interval (0,1], although the closer C_r is to 1, the better the simulation is, however within a small range close to 1, it is not in line with this rule. As shown in the following table.

TABLE 5 VARIATIONS IN PARAMETERS WITH DIFFERENT U

u **(m/s)**	Δt **(s)**	**Parameters**				
		C_r	D_n	D_x	$D_x - D_n$	%
0.2	999.5	0.9995	0.01	0.025298	0.0153	60.48
0.5	399.5	0.99875	0.0625	0.063246	0.0007	1.11
0.8	249.5	0.998	0.16	0.101193	-0.0588	58.11
1.0	199.5	0.9975	0.25	0.126491	-0.1235	97.64

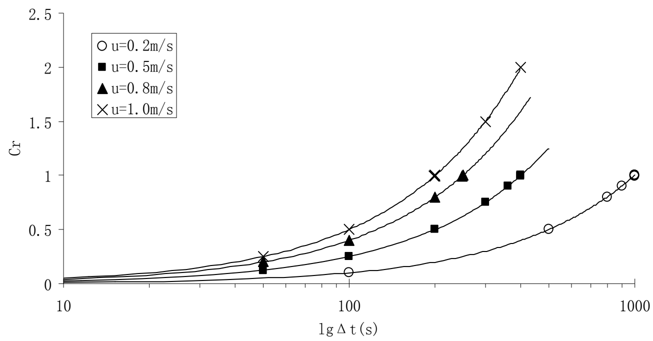

FIG. 1 DISTRIBUTION OF C_r WITH GROWTH OF THE TIME STEP Δt (IN LOG FORM)

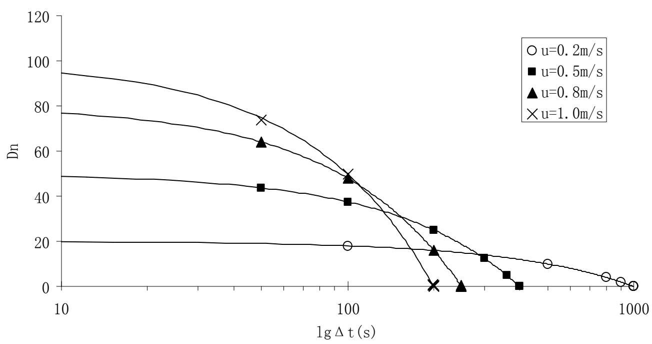

FIG. 2 DISTRIBUTION OF D_n WITH GROWTH OF THE TIME STEP Δt (IN LOG FORM)

Obviously, in the descending process of u , C_r is getting closer to 1, but $D_x - D_n$ is then minimum when u =0.5m/s. The existence of a smaller difference can be

tested by changing the value of u, however it is no longer studied here.

In fact, in order to get the parameters conditions of numerical diffusion that accurately simulate physical diffusion, formulas are used to reason reversely, assume $D_x = D_n$

We get:

$$D_n = \frac{u\Delta x - u^2\Delta t}{2} = D_x = 0.25u_* h = 0.25\sqrt{g}\frac{u}{C}h$$

Simplify it to be:

$$\Delta x = u\Delta t + \frac{0.5\sqrt{g}h}{C}$$

By assuming $k = \frac{0.5\sqrt{g}h}{C}$, we can obtain:

$$\Delta t = \frac{\Delta x - k}{u}$$

Obviously, Δt is a linear function of Δx, where k is a constant related to the parameters of the physical model. Take u =0.5, h =4, C =25, Δx =200m into the formula then the calculation shows Δt =399.499 which is very close to the above 399.5, so the difference between the two diffusion coefficients is insignificant. But this step size is very unfavorable to calculation; as it is tendency to take an integer as much as possible. Although in different engineering cases, different parameters of the physical model can improve the value of Δt, its value depends completely on the differential scheme itself. In order to keep the generality, the following will horizontally contrast a variety of commonly used differential schemes under the current model parameter conditions to examine whether a scheme can achieve a relatively satisfying step value.

Comparison among Various Difference Schemes

Although various differential schemes have different compatibility and stability conditions, as long as extracting numerical diffusion coefficient after dispersing pure convection equations respectively, then equivalent unify with the physical diffusion coefficient, we can obtain the calculation formula for step size (Table 6).

Obviously, these three schemes of Dobbins, Upwind and implicit have the same method to select the step size, and they also have the same characteristics represented by the Upwind scheme. The low-order Preissmann scheme is more suitable for the large stride length, and the possibility of an integral step length has been improved in this way, where φ =0.6, θ =0.4, Δt =19900s, and D_n =0.05, which shows a difference of 20.94% with D_x. When Δt =19870s and D_n =0.065, D_n show a difference of 2.77% with D_x and precision can meet the requirements. Instead, Lac-Friedrichs scheme is more suitable for small time step. Though the step is smaller, the simulation accuracy is not improved, such as when Δt =247s and D_n =0.097, Δt is only 0.1s smaller than 247.1s, while the relative error of diffusion coefficient reaches an unsatisfactory level, 52.83%.

TABLE 6 RESULTS OF DIFFERENT CALCULATION FORMULATIONS

Scheme name	D_n expression	Δt expression	Calculation results
Dobbins	$\frac{\Delta x^2 C_r(1-C_r)}{2\Delta t}$	$\Delta t = \frac{\Delta x - k}{u}$	399.5
Upwind	$\frac{\Delta x^2 C_r(1-C_r)}{2\Delta t}$	$\Delta t = \frac{\Delta x - k}{u}$	399.5
Implicit	$\frac{\Delta x^2 C_r(1+C_r)}{2\Delta t}$	$\Delta t = \frac{k - \Delta x}{u}$	-399.5
Preissmann	$\frac{\Delta x^2 C_r(2\varphi-1)}{2\Delta t} + C_r(2\theta-1)$	$\Delta t = \frac{k\Delta x + (1-2\varphi)\Delta x^2}{2(2\theta-1)}$	19874.8① 20125.2②
Lac-Friedrichs	$\frac{\Delta x^2(1-C_r-C_r^2)}{2\Delta t}$	$\Delta t = \frac{\sqrt{5\Delta x^2 + 2k\Delta x - k^2} - k - \Delta x}{2u}$	247.1

Note:

1. In the table $k = 0.5\sqrt{(gh)}/C$, where h =4m, Chezy coefficient C =25, flow rate u =0.5m/s, Δx =200m;
2. Preissmann scheme only consider the low-order condition, i.e. φ, θ is not equal to 0.5, ①, ②, are respectively corresponding to the different values of φ, θ, where ① is corresponding to φ =0.6, and θ =0.4, ② is corresponding to φ =0.4, and θ =0.6.

Conclusions

The paper starts from Upwind scheme, stating the process that generates numerical diffusion when dispersing suspended load convection-diffusion equation with a low-level difference scheme, and it tries to simulate the physical diffusion phenomenon using numerical diffusion, simulation accuracy under different parameters, such as Δt , Δx and u , are calculated. And by horizontally comparing different differential schemes we can get the following conclusions:

1) Numerical diffusion of differential scheme can be used to simulate the actual physical diffusion phenomenon, but it has certain requirements on the parameter selection. For suspended load convection-diffusion equation, the simulation method is to disperse the pure convection equation first, and then propose diffusion term. Since the coefficient in front of diffusion term is the numerical diffusion coefficient, by assuming which equals to the physical diffusion coefficient, we can get the relationship equation composed of some parameters that meet the simulation accuracy.

2) In general, in the various parameters, only spatial interval Δx and time step Δt which are related to the calculation can be chosen randomly, and the selection of Δx needs to be compatible with the size of the project and the complexity of the boundary, so the key is the time step Δt . By calculation, this paper has found the relationship of Δt that meets the accurate simulation under various differential schemes, but usually the calculated step sizes are with decimals, which is not conducive to calculation, so an instance is used to calculate the relative error between the numerical diffusion coefficient and the physical diffusion coefficient when Δt takes a similar integer value. It is found that as the step of low-level Preissmann scheme is larger, the possibility of an integral step is greatly increased, thereby increasing the calculation accuracy, which is a recommended method.

3) Though this article only analyzed suspended load convection diffusion equation, it can be speculated that bedload convection-diffusion equation, as well as the convection-diffusion phenomena of pollutants in the water, can be analyzed using the same method. Similarly, the method can be employed to solve the general problems by means of its unique superiority of differential equations - clear mathematical foundation, simple calculation and easy programming, which is still favourably compared to a more precise numerical method.

REFERENCES

Gasiorowski D. “Balance Errors Generated by Numerical Diffusion in the Solution of Non-linear Open Channel Flow Equations.” Journal of Hydrology 476 (2013): 384-394.

Papadakis Antonis P., and Metaxas Andrew C. “Optimum Mesh Dependent Diffusion Coefficient Proof from High to Low Order Upwind Schemes Utilized in Plasma Discharges.” 10th WSEAS International Conference on EHAC'11 and ISPRA'11, 3rd WSEAS Int. Conf. on Nanotechnology, Nanotechnology'11, 6th WSEAS Int. Conf. on ICOAA'11, 2nd WSEAS Int.Conf. on IPLAFUN'11, 2011.

Richard Courant, Kurt Otto Friedrichs, and Hans Lewy. “On the Partial Difference Equations of Mathematical Physics.” Math. Ann. 100 (1928): 32.

Xie Jianheng. Rivers Simulation. Beijing: Water Power Press, 1990.

Yang Guolu. Rivers Mathematical Model. Beijing: Ocean Press, 1993.

Zheng Bangmin, and Zhao Xin. Calculation of Water Dynamics. Wuhan: Wuhan University Press, 2001.